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The initial stages of growth of Ge on Si(001) studied by x-ray diffraction

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Abstract. The structure of an ultra-thin epitaxial Ge layer during *in situ* deposition onto a Si(001) surface has been investigated. Peaks arising from the 2×1 reconstruction disappear at a coverage of ≈ 3 ML. The layer is epitaxial with respect to the substrate up to a coverage of ≈ 5 ML, beyond which the strained layer relaxes gradually. At a coverage of 10 ML the lateral strain is reduced to 2.2% compared with 4.0% in the unrelaxed layer.

Epitaxial germanium layers may be grown on the Si(001) surface in a layer-by-layer mode up to a critical thickness of 6 ML [1]. Grazing-incidence x-ray diffraction at the Daresbury synchrotron has been used to investigate quantitatively strain relief and reconstruction during *in situ* deposition onto a clean Si(001) substrate at a temperature of 500 °C.

The (1.5, 0, 0.02) and (0, 1.5, 0.02) fractional-order peaks, arising from the double-domain 2×1 reconstruction, were monitored as a function of coverage θ . Their intensity was greater at $\theta = 1$ ML than for the clean surface, indicating that the reconstruction involves dimerisation of the heavier Ge atoms. The peak width was unchanged at both

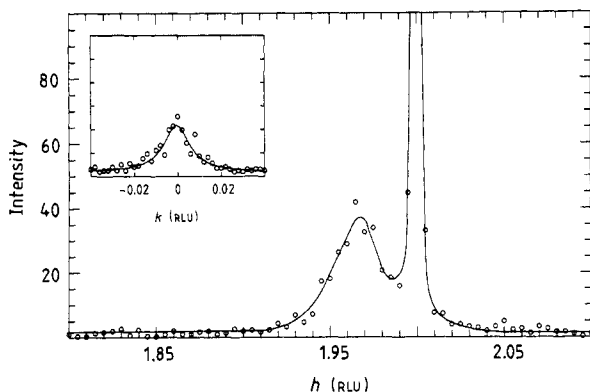


Figure 1. A radial scan through the (2, 0) Bragg peak for $\theta = 10$ ML. The inset shows a transverse scan at (1.965, 0).

coverages corresponding to an average reconstructed domain size of 3800 Å. For $\theta = 2$ ML and 3 ML the peak became much weaker and the domain size decreased to 2200 Å. The reconstruction was not observed at higher coverages, in agreement with LEED data [2].

Radial scans in reciprocal space through the (2, 0) Bragg peak, at the critical angle of incidence of 0.20° for which the penetration is ≈ 30 Å, were used to quantify strain relief. The peak from the Ge layer superimposed on that of the underlying Si up to $\theta = 5$ ML. This indicates that the layer is epitaxial with the substrate, the lateral strain of $(4.0 \pm 0.4)\%$ not being appreciably reduced. At $\theta = 7$ ML the peak is shifted, the strain being $(3.4 \pm 0.4)\%$, and at $\theta = 10$ ML the strain is $(2.2 \pm 0.3)\%$ (figure 1). The Ge layer is thus not fully relaxed at this coverage. A transverse scan through the Ge peak displayed a Lorentzian profile, indicative of exponentially decaying correlations. The peak width corresponds to a correlation length of 85 Å (figure 1). If it is assumed that this peak is due to islands of Ge, which have been observed with SEM for $\theta = 20$ ML [3], then average lateral dimensions of ≈ 200 Å are obtained.

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